Atmospheric Plume Modeling of Class 2 Liquefied Compressed Gases

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Creating a Three-Dimensional Simulation of Atmospheric Hazardous Chemical Dispersion

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Abstract

In order to aid Virginia's Office of Homeland Preparedness, the 2004 NASA DEVELOP Homeland Security team used existing plume modeling technology to simulate a chemical release. Richmond, Virginia was selected as the site of a potential plume point source due to its government connection and its potential vulnerability as a political and economic target. The plume dispersion point source was positioned at a vital railroad-interstate junction (identified by geographic coordinates) based on infrastructure assessment and demographic information. Additionally, the locations of industrial plants in the surrounding area are believed to be susceptible targets and therefore support the selection of this release point.

The Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT 4.7) model was used to simulate a hypothetical atmospheric dispersion of an immediate release of ammonia, chlorine, propane, and vinyl chloride. This model, designed by the National Oceanic and Atmospheric Administration (NOAA) in collaboration with the Australian Bureau of Meteorology, maps the movement of an air parcel (plume) through coupling of wind trajectories and meteorological information. NASA and NOAA observation sources provide input data to HYSPLIT 4.7.

These simulations were conducted in order to provide emergency personnel with a method that offers effective tracking of released hazardous chemicals. The results of this work prepare interactions with the Virginia Readiness, Response and Recovery Program and assist first responders in developing informative policies for crisis management in the event of a human-induced disaster.

Introduction

In the year 2000, 1.23 million tank cars containing hazardous materials were shipped in the United States. Sixty percent of these cars were built before 1989 from non-standardized steel (Conners 2004). The possibility of failure during the transport of these substances has sparked substantial concern regarding the preparedness of government agencies in the case of such an occurrence. When gases are released into the air, the particle cloud spreads and travels in conjunction with atmospheric conditions. By using various air trajectory and plume models, the path and spread of the particle cloud can be estimated. This plume modeling is the focus of NASA DEVELOP's 2004 Homeland Security project.

Hazardous class 2 liquefied compressed gases as identified by the U.S. Department of Transportation (DOT) comprise approximately twenty percent of all hazardous material shipments (Connors 2004). These gases include: ammonia, chlorine, propane, and vinyl chloride. Class 2 materials in seamless steel containers are frequently transported by truck and are vulnerable to attack during their course of travel. The regional dispersion of these gases following release was simulated in order to improve the Virginia Readiness, Response and Recovery Program (VR3) of the Virginia Geographic Information Network (VGIN).

Likewise, the Commonwealth of Virginia's Office of Homeland Preparedness has focused its efforts on the release of chemical and radioactive materials in the vicinity of Richmond, Virginia, chosen for its population and political significance. Designed to improve public preparedness in the case of an unanticipated terrorist attack, the VR3 program subsequently provides a plan for recovery and emergency aid. Researchers have joined forces with DOT to evaluate the vulnerabilities facing the transportation industry in the shipping of chemical substances, and millions of dollars have been budgeted for this program and other first response initiatives throughout the state of Virginia (News 1).

After comparing several plume models, the HYbrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model, version 4.7, was selected as most suitable for the needs of this project. Unlike other commercially available plume modeling programs, HYSPLIT 4.7 allows better regional tracking of particle dispersion by taking into account the varying terrain and atmospheric changes present in an urban environment. A popular model for calculating pollutant concentration and spread is the Gaussian plume model. Based on Gauss' advection-diffusion equation, this model assumes that dispersion in both the horizontal and vertical directions takes the shape of the Gaussian normal curve centered about the point source with a standard deviation that is an increasing function of time and downwind distance. The model was run on one-hour averages using ammonia, chlorine, propane, and vinyl chloride for a simulated nine-hour span. From these runs, a series of three-dimensional visuals were assembled to show the range of dispersal and the change in chemical concentration as the plume spread. Ultimately, the HYSPLIT 4.7 model depicted the computer-generated dispersal of class 2 liquefied compressed gases in order to better understand the urban travel of hazardous materials and assist first response emergency personnel in predicting where they might concentrate their rescue efforts.

Background

By incorporating National Weather Service (NWS) forecasts of wind direction, wind speed, cloud cover, and cloud ceiling, the HYSPLIT model is able to overcome some of the limitations of the simple Gaussian model. Variable wind speeds, complex topography, and wind shear were all considered in the final dispersion outputs produced by this HYSPLIT simulation. The NWS' National Centers for Environmental Prediction (NCEP) runs Eta Data Assimilation System (EDAS), an operational system for computer analyses and forecast. Several fields, including u- and v-wind components, temperature, and humidity, are contained in the EDAS archive. This data provided the meteorological input for the HYSPLIT model.

Land cover data and terrain information for the 3-D visuals came from the Enhanced Thematic Mapper Plus (ETM+) instrument on board the NASA Landsat 7 satellite, launched on April 15, 1999. The NASA Terra mission and Shuttle Radar Topography Mission (SRTM) also provided visual information via its digital imaging of terrain elevation. High-resolution digital orthophotography obtained from the Virginia Geographic Information Network was used to visualize the urban terrain of the dispersion point source. One foot and two foot resolutions were used in this data.

Class 2 liquefied compressed gases are identified as both flammable and corrosive materials. When dispersed, they may cause anywhere from temporary to lasting medical conditions. Quick evaporation rates make the gases dangerous to organism tissue and may lead to frostbite. An atmospheric release of ammonia gas would dictate the evacuation of all inhabitants surrounding the release area. Ammonia is reported to cause severe respiratory irritation upon exposure as well as damage to victims' vision. Skin irritation may also occur. Chlorine spills can lead to chronic health problems as well as immediate effects like burning, impaired vision, and corrosion to the respiratory tract. As propane is a noted flammable liquid, a release may be easily ignited upon mixture with oxygen. Liquid petroleum gas is also subject to ignition, and exposure victims may also expect respiratory irritation. Effects vary from headaches and nausea to unconsciousness. Vinyl chloride shares similar characteristics with the previous gases. Acting as an anesthetic in concentrated doses, individuals within the immediate dispersion range may experience drowsiness and numbness (MSDS 2004).

Results/Discussion

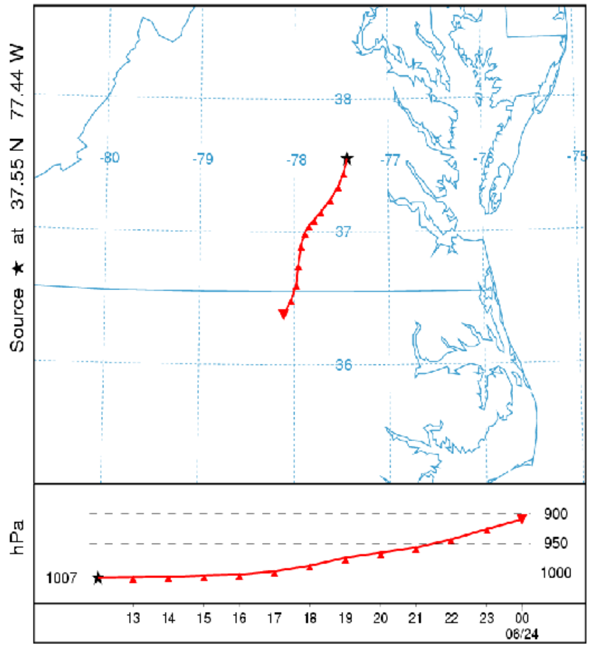

Figure 1: Forward wind trajectory plot from NOAA HYSPLIT air trajectory model.

Figure 1 shows the point source of chemical release positioned in Richmond, Virginia at the coordinates: 37.55°, -77.44°. Outputs from the NOAA HYSPLIT model show a graphical depiction of dispersing atmospheric plumes along an allotted time's forward wind trajectory. From the plume point source, the wind travel for the specified hours of sampling was monitored and placed upon an air trajectory plot via the NOAA HYSPLIT program. Figure 1 is a display of the NWS' archived wind travel plot for the morning hours of June 23, 2004. Release sampling began at 12:54 (Universal Time Clock) and was discontinued at 21:54. The figure shows the air travel relative to distance as well as the surrounding air pressure as it relates to the elapsed sampling hours. At the time of release, standard temperature and pressure conditions were recorded by the NWS archives. These conditions were advantageous since they resemble those simulated in the lab. The gases thus exhibited properties similar to those recorded at standard conditions.

The series of illustrations uses color shadings to monitor the change in molar concentration over time relative to position. Figure 2 features an atmospheric dispersion of ammonia released from a point source in Richmond, Virginia indicated by the outlined star. The plume was designed using the HYSPLIT incorporation of the Gaussian puff particle program. This program uses atmospheric chemistry to estimate the changes in concentration as the plume travels. Upon the immediate release area seen in Figure 2a, concentrations reach levels of 10^5 molar. As the plume travels and increases in volume, molarity begins to decrease with time. Samples from the model were graphed with Figure 2a representing the first hour after dispersion, 2b the third hour, 2c the sixth hour, and 2d the ninth and final hour of monitoring. Although the figures on the right are shown at three-hour intervals, the sample was

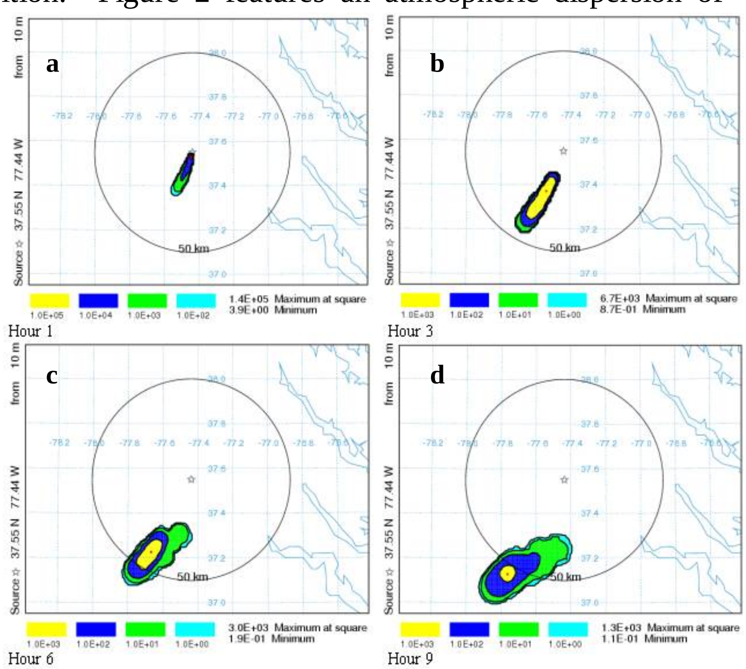

Figure 2: Ammonia dispersion as monitored by NOAA HYSPLIT 4.7 . Three-hour measurements are shown along with corresponding molar concentration shading.

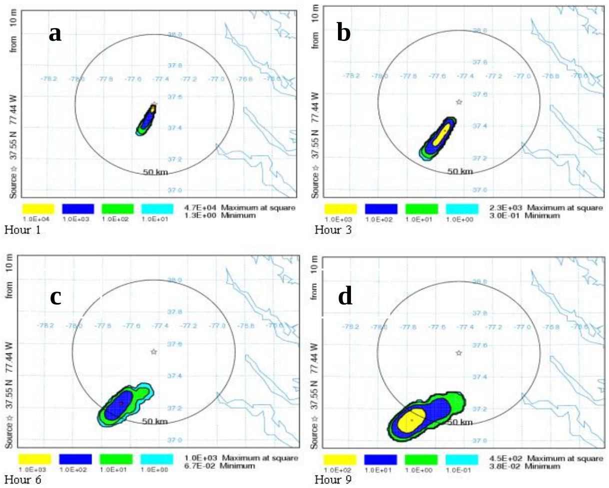

Figure 3: Chlorine outputs from the NOAA HYSPLIT 4.7.

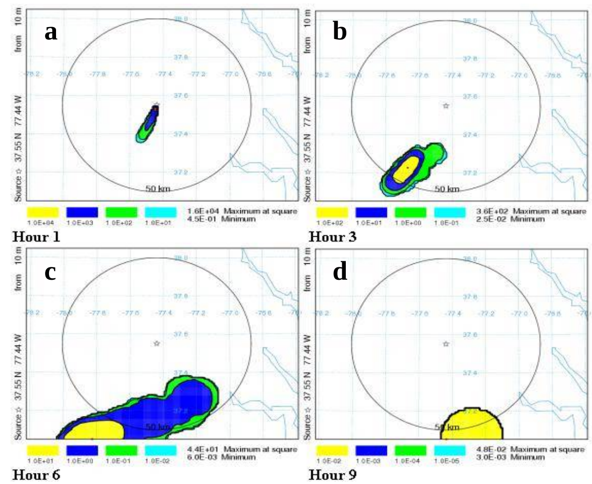

Figure 4: Propane release from the NOAA HYSPLIT 4.7.

monitored at hourly intervals. These grids were representative of measurements taken in the horizontal direction at a vertical distance of 50m. Variable vertical measurements up to 12km were also taken and a minimal change in concentration was found.

The physical properties of chlorine gas were applied in the parameters of the HYSPLIT model. Like the ammonia release, the chlorine plume (Figure 3) traveled along the same air trajectory and followed the same spread pattern. Since chlorine is a more reactive gas, the concentration analysis varied in concentration intensity.

Dispersions of propane and vinyl chloride were also graphed showing both position and concentration in Figures 4 and 5. While all graphs may appear similar, their molar intensity fluctuates with position. This variation comes from the reactions within the HYSPLIT model that determine the change in local and long-range atmospheric chemistry.

Population density measurements were then coupled with the HYSPLIT generated plumes in order to show the potential effect on area citizens (Figure 6). Census information from the year 2000 was compiled according to zip code districts in the Richmond area as well as by counties surrounding the city. These graphical representations were later included

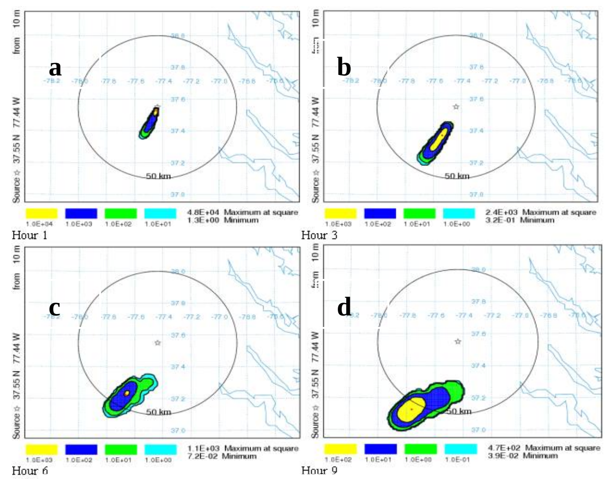

Figure 5: Vinyl chloride outputs from the NOAA HYSPLIT 4.7.

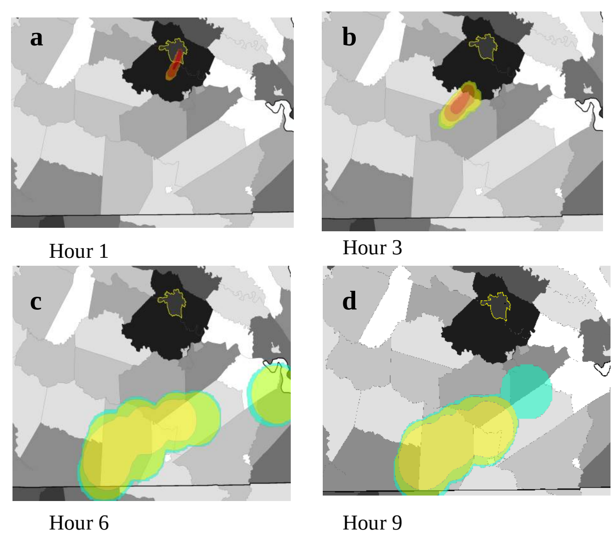

Figure 6: Ammonia plume dispersal graphed over Virginia population density per county.

in a 3-D visualization. The plume was displayed over high-resolution digital orthophotography provided by VGIN under strict user agreement. The orthophotography at one-meter resolution enabled a detailed depiction of Richmond's urban terrain. These visuals contributed to the final release analysis.

The results from this project are beneficial in illustrating the potential effects of a chemical release in an urban environment. A run time of nine hours was used in order to maintain a regional view of the traveling plume so that the model's output would be valuable to policy makers and emergency personnel in assessing the needs of a targeted area. A greater understanding of these trajectories suggests the possibility of improved decision-making in emergencies. HYSPLIT's versatility ensures its value as a program that can be used from any geographic location for both local and long-range assessment. Archived meteorological data within the model allows a clearer focus on the chemical dispersion rather than exhausting resources in the collection of weather data.

Due to the human and economic expenses of these studies, a computer-generated simulation provides a more cost-efficient testing ground for potential environmental dispersions. This study's outcome is significant because it creates a foundation for further investigation into the atmospheric modeling of class 2 liquefied compressed gases released in large volumes. Information on these potential releases can be catalogued and compared to those simulated through other dispersion models. Coupled with HAZMAT information, model predictions may be used to estimate the affect of simulated dispersals on surrounding communities.

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